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RAILCAR SENSITIVITY ANALYSIS

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ASYMMETRIC SYSTEMS DEPARTMENT

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This sensitivity analysis was designed to determine how certain input parameters would affect the output parameters of the RAILCAR computer program, a tool used to predict the physical characteristics of a toxic industrial chemical (TIC) release from a transport container. Three vignettes (evaporating liquid pool, boiling liquid pool, stationary vapor cloud) were studied; parameters were identified for each that significantly affected the output source characterizations. While some input parameters only had an influence on one vignette, others affected all three. Hole diameter and boiling temperature had significant effects on all three vignettes, but tank pressure, critical temperature, and vapor density did not affect any of the output parameters (within the scope of this analysis).

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FOREWORD

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This report has been reviewed by Gaurang R. Davë, Head, CBR Analysis, Testing & Systems Engineering Branch (Code Z24), and Michael Purello, Head, CBR Defense Division.

Approved by:

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1.0 INTRODUCTION

The RAILCAR Program is a tool used to predict the physical characteristics of a toxic industrial chemical (TIC) release from a transport container. The inputs to the program characterize the conditions inside the container and the characteristics of the environment in which the TIC is released. Based on the input parameters, the program calculates the physical properties of the chemical release. The purpose of this sensitivity analysis is to determine which input parameters have the greatest influence on the source characteristics for three different vignettes. The vignettes represent chemicals with low, medium, and high volatility producing an evaporating liquid pool, a boiling liquid pool, and a stationary cloud respectively.

Two files are used to deliver the input parameters to the RAILCAR program. The first is a .DAT file, which contains information about the conditions inside the container and of the outside environment. Physical characteristics of the container, such as wall thickness and the size of the hole, are stored in this file. The other file, RAILCAR.PAR, contains thermodynamic information on each of the TICs available in the program. Both of these files were used in this study. For more information on the program development and a full description of all the input parameters, see the RAILCAR Users' Manual.

2.0 METHODS

The one-factor-at-a-time (OAT) sensitivity analysis method was used for this study. Each input parameter was varied from a baseline value while all other input parameters were held constant. This shows how an individual input parameter affects the program's output parameters. Each parameter was evaluated at three values: the baseline, a 25% decrease from the baseline value (75% of baseline), and a 25% increase from the baseline value (125% of baseline). For the ±25% variances, the output was then compared to the baseline output values and a percentage difference calculated by Equation (1).

$$\%Difference = \frac{OutputValue - BaselineValue}{BaselineValue} * 100 \qquad (1)$$

The first step was to establish the baseline input sets for each of the three vignettes. It was important that the baseline values were not the maximum or minimum values for that particular parameter. This would allow them to be varied by ±25% for the study. For example, the pool mass fraction absorbing into the ground must be between 0 and 1; therefore, in order to study the effects on that parameter, 0 or 1 could not be chosen for the baseline. Output files generated by the baseline inputs using RAILCAR4 were compared to output files that represented the three volatility cases from a previous version of the RAILCAR program. The main goal was to accurately represent the physical characteristics of the three vignettes: evaporating liquid pool, boiling liquid pool, and stationary cloud. Once reasonable agreement between the old and new output files was reached, the corresponding set of input parameters was set as the baseline.

Next the trade space was established. Each input parameter was varied by ±25% of the baseline value. Input parameters included values from the .DAT file as well as the TIC thermodynamic properties located in the RAILCAR.PAR file. In total, 36 input parameters were included in the study. Input parameters and thermodynamic properties are listed below in Tables 1 and 2. Table B-1 in Appendix B shows the trade space and baseline values for the three vignettes.

Table 1: RAILCAR Input Parameters

initial tank mass	inert head pressure	pool depth
recovered mass	ullage volume fraction	pool mass absorbed into ground
air temperature	aerosol fraction	entrainment ratio
ground temperature	tank thickness	cloud height
tank temperature	hole diameter	friction velocity
humidity	orifice diameter	wind speed
tank pressure	liquid fraction foam	sheltering factor
liquid head pressure	minimum vaporization fraction	

Table 2: TIC Thermodynamic Properties

freezing temperature	critical temperature
molecular weight	liquid viscosity
liquid heat capacity	vapor heat capacity
liquid surface tension	vapor diffusivity
liquid density	liquid density rate
boiling temperature	heat of vaporization
heat of vaporization rate	

One parameter, that was not an explicit input value, was the boiling temperature. This value was varied by ±25% by changing the values of the Antoine equation constants in the RAILCAR.PAR file. The Antoine equation is as follows:

$$\log_{10} p = A - \frac{B}{C+T} \tag{2}$$

Where p is the pressure, T is the temperature, and A, B, and C are the Antoine constants. The boiling temperature is calculated from this equation at a pressure of 1 atm. Replacing p with 1 atm, a simpler relationship between temperature and the constants can be found

$$T = \frac{B}{A} - C \tag{3}$$

T became the known quantity (±25% of baseline value) so the constants A, B, and C were varied to achieve the desired value of T.

Once the trade space was established, .DAT files were created and run through the RAILCAR program. Raw output data were recorded in an Excel sheet for each vignette. The numerical data was then converted to a percentage difference from the baseline value. The baseline output data for each vignette are given in Tables B-2 through B-4 in Appendix B. The following section discusses the results obtained from the analysis.

3.0 RESULTS

Percentage changes of the output parameters were calculated from the baseline values using Equation (1). An input parameter's influence on an output parameter was categorized based on the percentage change values. The categories are described in Table 3.

Table 3: Influence Category Definition

Impact	Absolute Value of Percentage Change (P)	Color
None	0	Blue
Low	$0<P\leq 25$	Green
Moderate	$25<P\leq 50$	Yellow
High	$P>50$	Red

NOTE: If a pair of values appears after an output parameter, those correspond to the 25% decrease and increase, respectively, of the input variable. Example: "tank temperature affects the following output parameters: liquid empty time (65, -91%)…" means that a 25% decrease in the tank temperature increased the liquid empty time by 65% and a 25% increase in tank temperature resulted in a 91% reduction in the liquid empty time.

3.1 Low Volatility – Nitric Acid

The spillage from a low-volatility TIC is characterized by the formation of an evaporating liquid pool. Low-volatility TICs have a high boiling point; as the liquid escapes the container, it does not become vaporized. Instead, if forms a pool that evaporates over time. Depending on the characteristics of the environment, some of the chemical will also absorb into the ground. The chemicals absorbed into the ground can continue to off-gas after the liquid pool has evaporated. Nitric acid was chosen as the low-volatility TIC.

For this vignette, the input parameter that had a significant effect on the output was the hole diameter. A 25% decrease in the baseline hole diameter increased the tank empty time and liquid empty time by 78%. For a 25% increase, the liquid jet flow rate and average jet flow rate increased by 56%. Table 4 summarizes the influence of varying the hole diameter on selected output parameters.

Table 4: Effect of Hole-Diameter Variation on Selected Output Parameters for the Low-Volatility TIC

Output Parameter	25% Decrease in Hole Diameter	25% Increase in Hole Diameter
Liquid empty time	78	-36
Liquid jet flow rate	-44	56
Tank empty time	78	-36
Avg. jet flow rate	-44	56

The thermodynamic property that had the largest influence on the output was the boiling temperature. It affected depressurization pressure, pool duration, maximum pool mass rate, off-gassing duration, and average pool mass rate by as much as 136%. See Table 5 for the percent change values of the above-mentioned parameters.

Table 5: Effect of Boiling-Temperature Variation on Selected Output Parameters for the Low-Volatility TIC

Output Parameter	25% Decrease in Boiling Temp	25% Increase in Boiling Temp
Depressurization temperature	133	-56
Pool duration	-53	106
Maximum pool mass rate	136	-53
Off-gassing duration	-57	112
Average pool mass rate	130	-53

Other significant factors include: ground temperature, initial tank mass, and molecular weight. Table B-5 shows how the input parameters affected all the output parameters. The color coding described in Table 3 at the beginning of this section is used to categorize the influence of each parameter for easy visualization.

The following input parameters had no effect on the output parameters: tank pressure, ullage volume fraction, aerosol fraction rained out due to impaction, percent liquid fill becoming foam, minimum vaporization percent, entrainment ratio, cloud height, friction velocity, and sheltering factor. Thermodynamic properties from the .PAR file that did not affect the output results were: freezing temperature, critical temperature, liquid heat capacity, vapor heat capacity, liquid surface tension, vapor diffusivity, heat of vaporization, and heat of vaporization rate.

3.2 Medium Volatility – Methyl Bromide

The release of a medium-volatility TIC produces a boiling liquid pool. The release from the container is characterized by a vapor plume and a liquid jet. Large droplets form and rain out of the vapor cloud. For this case, RAILCAR calculates what percentage of the escaping chemical is vapor and liquid. From that information it then can determine the diameter of the vapor plume escaping the container, the characteristics of the liquid pool formed on the ground, and also the characteristics of the resulting vapor cloud. Methyl bromide was chosen as the TIC for the medium-volatility vignette.

Input parameters that had a significant impact on the results were the orifice diameter, hole diameter, tank temperature, and the minimum vaporization percent. Heat of vaporization was the thermodynamic parameter that had a major effect on the output. These input parameters primarily affected the following source characteristics: liquid empty time, liquid jet flow rate, tank empty time, average jet flow rate, plume diameter, pool diameter, pool duration, maximum pool mass rate, off-gassing duration, and average pool mass rate. An excerpt from the full data table for methyl bromide (Table B-6) is shown below for the parameters described above.

Table 6: Effect of Significant Input Parameters on Selected Output Parameters for the Medium-Volatility TIC

	25% Decrease in:					**25% Increase in:**		
Input→ / Output	Tank Temp	Hole Diameter	Orifice Diameter	Min Fraction Vaporization	Heat of Vaporization	Tank Temp	Hole Diameter	Heat of Vaporization
Liquid empty time	15	78	300	-68	-64	-65	-36	-7
Liquid jet flow rate	-13	-44	-75	213	177	187	56	7
Tank empty time	8	78	207	-47	-40	-44	-36	-7
Avg jet flow rate	-8	-44	-67	87	67	79	56	7
Plume diameter	7	-26	-49	6	4	7	25	1
Pool diameter	-6	-25	-50	76	65	68	25	4
Pool duration	14	73	281	-64	-60	-61	-34	-6
Max pool mass rate	-12	-44	-75	209	173	182	56	7
Off-gassing duration	13	70	273	-61	-57	-58	-32	-6
Avg pool mass rate	-11	-41	-73	155	131	136	47	7

The final tank temperature was heavily influenced by the inert head pressure (-120, 134%), ullage volume fraction (-85, 80%), molecular weight (206, -105%), vapor heat capacity (223, -107%), and boiling temperature (119, -96%). These input parameters had little effect on the other output parameters. A moderate effect was seen on cloud temperature by the following input parameters: tank temperature (66, -26%), percent liquid fill becoming foam (-36, 44%), entrainment ratio (37, -26%), molecular weight (-25, 24%), liquid heat capacity (32, -18%), and heat of vaporization (-56, 74%).

The following input parameters had no effect on the output: ground temperature, tank pressure, liquid head pressure, aerosol fraction rained out due to impaction, tank thickness, pool mass fraction absorbing into the ground, friction velocity, and sheltering factor. The thermodynamic properties that had no effect were freezing temperature, critical temperature, and vapor diffusivity.

3.3 High Volatility – Hydrogen Sulfide

Hydrogen sulfide was chosen as the high-volatility TIC. A high-volatility TIC can be characterized by a low boiling temperature. When the TIC is released, it vaporizes and produces a stationary vapor cloud. Droplets that form in the cloud are too small to rain out onto the ground. RAILCAR calculates the size and duration of the vapor cloud.

The hole diameter had a significant effect on the output; liquid empty time, liquid jet flow rate, tank empty time, and average jet flow rate all experienced significant percentage changes with ±25% changes from the baseline. Table 7 below shows this.

Table 7: Effect of Hole-Diameter Variation on Selected Output Parameters for the High-Volatility TIC

Output Parameter	25% Decrease in hole diameter	25% Increase in hole diameter
Liquid empty time	78	-36
Liquid jet flow rate	-44	56
Tank empty time	78	-36
Avg jet flow rate	-44	56

Depressurization temperature was greatly impacted by initial tank mass (59, -36%), ullage volume fraction (61, -68%), and tank temperature (-215, 214%) while having a low to moderate impact on the other output parameters. Depressurization temperature was also greatly affected by the following thermodynamic properties: molecular weight (221, -204%), liquid heat capacity (-261, 171%), liquid density (-313, 184%), boiling temperature (-328, 300%), and heat of vaporization (281, -254%). Table B-7 in Appendix B shows the complete results for hydrogen sulfide.

Ground temperature and tank pressure had no effect on the RAILCAR output parameters. The thermodynamic properties of critical temperature and vapor diffusivity did not affect the output parameters either.

3.4 All Vignettes

This section will describe parameters that had a common influence on all three volatility cases. Input parameters that had a moderate to significant effect on output for all three vignettes were:

- Hole diameter: affected liquid empty time, liquid jet flow rate, tank empty time, and average jet flow rate for all three vignettes
- Orifice diameter: had a significant effect on the medium-volatility vignette, moderate to low effect on the other two vignettes
- Initial tank mass: moderate effect for all three vignettes
- Boiling temperature
- Molecular weight

Tank pressure, the critical temperature, and the vapor density had no effect on any of the output parameters within the scope of this study. Other factors that had minimal effect on the results, in increasing order, are: tank thickness, liquid head pressure, humidity, air temperature, liquid viscosity, and liquid surface tension.

4.0 CONCLUSION

The purpose of this sensitivity analysis was to determine how the input parameters affected the output parameters of the RAILCAR program. Three vignettes were studied, each having different physical output characteristics (evaporating liquid pool, boiling liquid pool, stationary vapor cloud). For each vignette, parameters were identified that had significant effects on the output source characterizations. While some input parameters only had an influence on one vignette, others affected all three. A summary of input parameters that had significant effects on each of the vignettes is given below:

- Low Volatility – Nitric Acid
    - Hole diameter
    - Boiling temperature
- Medium Volatility – Methyl Bromide
    - Hole diameter
    - Orifice diameter
    - Minimum vaporization percent
    - Tank temperature
    - Heat of vaporization
- High Volatility – Hydrogen Sulfide
    - Hole diameter
    - Boiling temperature

Hole diameter and boiling temperature had significant effects for all three vignettes. On the other hand, tank pressure, critical temperature, and vapor density had no effect on any of the output parameters within the scope of this analysis.

APPENDIX A

ABBREVIATIONS USED IN COMPREHENSIVE DATA TABLES

ABBREVIATIONS USED IN COMPREHENSIVE DATA TABLES

af	aerosol rainout fraction due to impaction
at	air temperature
bt	boiling temperature
ch	cloud height
ct	critical temperature
er	entrainment ratio
ft	freezing temperature
fv	friction velocity
gt	ground temperature
h	humidity
hd	hole diameter
hov	heat of vaporization
hovr	heat of vaporization rate
ihp	inert head pressure
itm	initial tank mass
ld	liquid density
ldr	liquid density rate
lff	percent liquid fill becoming foam
lhc	liquid heat capacity
lhp	liquid head pressure
lst	liquid surface tension
lv	liquid viscosity
mfv	min fraction vaporization
mw	molecular weight
od	orifice diameter
pd	pool depth
pma	pool mass absorbed
rc	recovered mass
sf	sheltering factor
t	tank thickness
tp	tank pressure
tt	tank temperature
uvf	ullage volume fraction
vd	vapor diffusivity
vhc	vapor heat capacity
ws	wind speed

APPENDIX B

COMPREHENSIVE DATA TABLES

Table B-1: Trade Spaces for All Vignettes

	NITRIC ACID			METHYL BROMIDE			HYDROGEN SULFIDE		
RAILCAR INPUT	-25%	Baseline	+25%	-25%	Baseline	+25%	-25%	Baseline	+25%
TIC		nitric acid			methyl bromide			hydrogen sulfide	
mass input type		2			2			2	
initial tank mass	33715.5	44954	56192.5	94882.5	126510	158137.5	21393.75	28525	35656.25
recovered mass	10114.5	13486	16857.5	9488.25	12651	15813.75	2139.75	2853	3566.25
air temp	19.5	26	32.5	6	8	10	6	8	10
ground temp	19.5	26	32.5	6	8	10	6	8	10
tank temp	19.5	26	32.5	6	8	10	6	8	10
humidity	50	75	100	45	60	75	45	60	75
tank pressure	0.75	1	1.25	0.75	1	1.25	0.75	1	1.25
liquid head pressure mode		2			2			2	
liquid head pressure	0.17925	0.239	0.29875	0.2895	0.386	0.4825	0.1215	0.162	0.2025
inert head pressure	0.75	1	1.25	0.75	1	1.25	0.75	1	1.25
ullage volume fraction	0.15	0.2	0.25	0.15	0.2	0.25	0.15	0.2	0.25
aerosol fraction	0.225	0.3	0.375	0.225	0.3	0.375	0.075	0.1	0.125
tank thickness type		2			2			2	
tank thickness	0.093	0.124	0.155	0.093	0.124	0.155	0.093	0.124	0.155
hole parameter type		1			1			1	
hole diameter	2.25	3	3.75	3	4	5	4.5	6	7.5
orifice type		2			2			2	
orifice diameter	2.25	3		3	4		4.5	6	
foaming		2			2			2	
liquid fraction foam	4.875	6.5	8.125	6.75	9	11.25	4.875	6.5	8.125
min fraction vaporization	1.5	2	2.5	1.5	2	2.5	1.5	2	2.5
liquid pool depth	0.75	1	1.25	0.75	1	1.25	0.75	1	1.25
pool mass absorbed	0.1125	0.15	0.1875	0.1125	0.15	0.1875	0.1125	0.15	0.1875
entrainment ratio	135	180	225	112.5	150	187.5	15	20	25
cloud height	3	4	5	1.5	2	2.5	0.75	1	1.25
wind input type		1			1			1	
friction velocity	0.274725	0.3663	0.457875	0.274725	0.3663	0.457875	0.207375	0.2765	0.345625
2m wind speed	2.4	3.2	4	2.4	3.2	4	2.4	3.2	4
entrainment factor		3			3			3	
sheltering factor	2.25	3	3.75	2.25	3	3.75	2.25	3	3.75
.PAR INPUT									
TIC		nitric acid			methyl bromide			hydrogen sulfide	
freezing temperature	-30.45	-40.6	-50.75	-70.2375	-93.65	-117.0625	-61.725	-82.3	-102.875
critical temperature	375	500	625	145.5	194	242.5	75.15	100.2	125.25
molecular weight	47.2575	63.01	78.7625	71.205	94.94	118.675	25.56	34.08	42.6
liquid viscosity at 20 C	0.5475	0.73	0.9125	0.3	0.4	0.5	0.105	0.14	0.175
liquid heat capacity at boiling	1.0425	1.39	1.7375	0.6225	0.83	1.0375	1.5	2	2.5
vapor heat capacity at boiling	0.6375	0.85	1.0625	0.33	0.44	0.55	0.7725	1.03	1.2875
liquid surface tension at boiling	30.675	40.9	51.125	20.325	27.1	33.875	8.85	11.8	14.75
vapor diffusivity at 20 C	0.07875	0.105	0.13125	0.06075	0.081	0.10125	0.08625	0.115	0.14375
liquid density at boiling	999.675	1332.9	1666.125	1297.5	1730	2162.5	711	948	1185
liquid density rate of change w/ temp	-2.025	-2.7	-3.375	-2.025	-2.7	-3.375	-1.3335	-1.778	-2.2225
Antoine constants									
A	4.992	5.627	6.101	4.072	4.295	4.559	4.149	4.5289	4.772
B	1500	2003	2500	900	1087	1300	800	958.587	1100
C	239.01	273.15	307.29	218.58	249.8	281.03	238.53463	272.611	306.68768
boiling temperature	61.470769	82.812325	102.47889	2.441611	3.2849825	4.1202522	-45.717079	-60.950994	-76.176359
heat of vaporization at boiling	494.25	659	823.75	188.8875	251.85	314.8125	409.545	546.06	682.575
heat of vaporization rate of change w/ temp	-0.714	-0.952	-1.19	-0.474	-0.632	-0.79	-0.90075	-1.201	-1.50125

Table B-2: Baseline Output for Nitric Acid

final tank temp.=	-25.65	C
depress. temperature=	26	C
depress. pressure=	0.09	atm
liquid empty time=	2339.9	s
liquid jet flow rate=	13.4481	kg/s
tank empty time=	2339.9	s
avg. jet flow rate=	13.4481	kg/s
plume diameter=	0.08	m
pool diameter=	48.8	m
pool duration=	10188.9	s
max. pool mass rate=	3.0103	kg/s
off-gassing duration=	15729.3	s
avg. pool mass rate=	2.0006	kg/s
cloud diameter=	0	m
cloud temperature=	26	C
cloud duration=	0	s
cloud vap. mass rate=	0	kg/s
Area vapor source properties:		
diameter=	48.8	m
duration=	15729.3	s
vapor mass rate=	2.0006	kg/s

Table B-3: Baseline Output for Methyl Bromide

final tank temp.=	-1.2	C
depress. temperature=	6.51	C
depress. pressure=	1.3	atm
liquid empty time=	7556.3	s
liquid jet flow rate=	13.5164	kg/s
tank empty time=	11079	s
avg. jet flow rate=	10.2512	kg/s
plume diameter=	1.36	m
pool diameter=	23.77	m
pool duration=	8089.3	s
max. pool mass rate=	13.3056	kg/s
off-gassing duration=	8265.6	s
avg. pool mass rate=	12.1638	kg/s
cloud diameter=	235.05	m
cloud temperature=	-9.22	C
cloud duration=	0	s
cloud vap. mass rate=	0	kg/s
Plume vapor source properties:		
diameter=	1.36	m
duration=	11079	s
vapor mass rate=	10.2512	kg/s

Table B-4: Baseline Output for Hydrogen Sulfide

final tank temp.=	-65.11	C
depress. temperature=	0.8	C
depress. pressure=	10.78	atm
liquid empty time=	64.8	s
liquid jet flow rate=	346.1998	kg/s
tank empty time=	160.9	s
avg. jet flow rate=	159.1514	kg/s
plume diameter=	4.72	m
pool diameter=	14.59	m
pool duration=	651.2	s
max. pool mass rate=	2.2968	kg/s
off-gassing duration=	1065.1	s
avg. pool mass rate=	1.5586	kg/s
cloud diameter=	262.61	m
cloud temperature=	-79.39	C
cloud duration=	114.2	s
cloud vap. mass rate=	212.1587	kg/s
Plume vapor source properties:		
diameter=	4.72	m
duration=	160.9	s
vapor mass rate=	159.1514	kg/s

Table B-5: Percentage Change Results Visualization:
Low-Volatility Vignette – Nitric Acid

	25% Decrease from Baseline Input Parameters																							25% Decrease from Baseline Thermo Properties												
	itm	rc	at	gt	tt	h	tp	lhp	ihp	uvf	af	t	hd	od	lff	mfv	pd	pma	er	ch	fv	ws	sf	ft	ct	mw	lv	lhc	vhc	lst	vd	ld	ldr	bt	hov	hovr
final tank temp	0	0	0	0	21	0	0	0	-36	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
depress. Temp	0	0	0	0	-25	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
depress. Pressure	0	0	0	0	-33	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	133	0	0
liquid empty time	-36	11	0	0	-1	0	0	3	12	0	0	0	78	15	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	14	1	2	0	0
liquid jet flow rate	0	0	0	0	1	0	0	-2	-11	0	0	0	-44	-13	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-12	-1	-2	0	0
tank empty time	-36	11	0	0	-1	0	0	3	12	0	0	0	78	15	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	14	1	2	0	0
avg. jet flow rate	0	0	0	0	1	0	0	-2	-11	0	0	0	-44	-13	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-12	-1	-2	0	0
plume diameter	0	0	0	0	0	0	0	0	0	0	0	0	-25	-25	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
pool diameter	-19	5	0	0	0	0	0	0	0	0	0	0	-2	0	0	0	14	0	0	0	0	1	0	0	0	1	0	0	0	0	0	12	1	-3	0	0
pool duration	-5	1	1	34	0	0	0	0	2	0	0	0	10	2	0	0	-22	4	0	0	0	22	0	0	0	29	0	0	0	0	0	-18	-2	-53	0	0
max pool mass rate	-34	10	-1	-27	0	0	0	0	-1	0	0	0	-5	-1	0	0	31	0	0	0	0	-20	0	0	0	-24	0	0	0	0	0	25	2	136	0	0
off-gassing duration	-3	1	1	36	0	0	0	0	1	0	0	0	6	1	0	0	-23	-7	0	0	0	24	0	0	0	31	0	0	0	0	0	-19	-2	-57	0	0
avg pool mass rate	-34	10	-1	-27	0	0	0	0	-1	0	0	0	-6	-1	0	0	30	8	0	0	0	-19	0	0	0	-23	0	0	0	0	0	24	2	130	0	0
cloud diameter	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
cloud temp	0	0	0	0	-25	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
cloud duration	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
cloud vap mass rate	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Area vapor source props																																				
diameter	-19	5	0	0	0	0	0	0	0	0	0	0	-2	0	0	0	14	0	0	0	0	1	0	0	0	1	0	0	0	0	0	12	1	-3	0	0
duration	-3	1	1	36	0	0	0	0	1	0	0	0	6	1	0	0	-23	-7	0	0	0	24	0	0	0	31	0	0	0	0	0	-19	-2	-57	0	0
vapor mass rate	-34	10	-1	-27	0	0	0	0	-1	0	0	0	-6	-1	0	0	30	8	0	0	0	-19	0	0	0	-23	0	0	0	0	0	24	2	130	0	0

	25% Increase from Baseline Input Parameters																							25% Increase from Baseline Thermo Properties												
	itm	rc	at	gt	tt	h	tp	lhp	ihp	uvf	af	t	hd	od	lff	mfv	pd	pma	er	ch	fv	ws	sf	ft	ct	mw	lv	lhc	vhc	lst	vd	ld	ldr	bt	hov	hovr
final tank temp	0	0	0	0	-21	0	0	0	31	0	0	0	0		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
depress. Temp	0	0	0	0	25	0	0	0	0	0	0	0	0		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
depress. Pressure	0	0	0	0	33	0	0	0	0	0	0	0	0		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-56	0	0
liquid empty time	36	-11	0	0	1	0	0	-2	-9	0	0	0	-36		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-10	-1	-2	0	0
liquid jet flow rate	0	0	0	0	-1	0	0	2	10	0	0	0	56		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	11	1	2	0	0
tank empty time	36	-11	0	0	1	0	0	-2	-9	0	0	0	-36		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-10	-1	-2	0	0
avg. jet flow rate	0	0	0	0	-1	0	0	2	10	0	0	0	56		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	11	1	2	0	0
plume diameter	0	0	0	0	0	0	0	0	0	0	0	0	25		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
pool diameter	15	-5	0	-1	0	0	0	0	0	0	0	0	1		0	0	-10	0	0	0	0	-1	0	0	0	-1	0	0	0	0	0	-9	-1	0	0	0
pool duration	5	-1	-1	-24	0	0	0	0	-1	0	0	0	-5		0	0	22	-4	0	0	0	-14	0	0	0	-17	0	0	0	0	0	18	2	106	0	0
max pool mass rate	33	-10	1	34	0	0	0	0	1	0	0	0	2		0	0	-19	0	0	0	0	18	0	0	0	23	0	0	0	0	0	-17	-2	-53	0	0
off-gassing duration	3	-1	-1	-25	0	0	0	0	-1	0	0	0	-3		0	0	23	7	0	0	0	-15	0	0	0	-18	0	0	0	0	0	20	2	112	0	0
avg pool mass rate	32	-10	1	34	0	0	0	0	1	0	0	0	3		0	0	-19	-7	0	0	0	18	0	0	0	22	0	0	0	0	0	-17	-2	-53	0	0
cloud diameter	0	0	0	0	0	0	0	0	0	0	0	0	0		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
cloud temp	0	0	0	0	25	0	0	0	0	0	0	0	0		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
cloud duration	0	0	0	0	0	0	0	0	0	0	0	0	0		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
cloud vap mass rate	0	0	0	0	0	0	0	0	0	0	0	0	0		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Area vapor source props																																				
diameter	15	-5	0	-1	0	0	0	0	0	0	0	0	1		0	0	-10	0	0	0	0	-1	0	0	0	-1	0	0	0	0	0	-9	-1	0	0	0
duration	3	-1	-1	-25	0	0	0	0	-1	0	0	0	-3		0	0	23	7	0	0	0	-15	0	0	0	-18	0	0	0	0	0	20	2	112	0	0
vapor mass rate	32	-10	1	34	0	0	0	0	1	0	0	0	3		0	0	-19	-7	0	0	0	18	0	0	0	22	0	0	0	0	0	-17	-2	-53	0	0

Table B-6: Percentage Change Results Visualization:
Medium-Volatility Vignette – Methyl Bromide

	25% Decrease from Baseline Input Parameters																							25% Decrease from Baseline Thermo Properties												
	itm	rc	at	gt	tt	h	tp	lhp	ihp	uvf	af	t	hd	od	lff	mfv	pd	pma	er	ch	fv	ws	sf	ft	ct	mw	lv	lhc	vhc	lst	vd	ld	ldr	bt	hov	hovr
final tank temp	16	-11	0	0	-33	0	0	0	-120	-85	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	206	0	0	223	0	0	0	0	119	0	0
depress. Temp	1	-1	0	0	-30	0	0	0	1	1	0	0	0	0	-1	0	0	0	0	0	0	0	0	0	0	5	0	-8	0	0	0	-8	0	-1	5	0
depress. Pressure	1	-1	0	0	-6	0	0	0	-3	-3	0	0	0	0	-1	0	0	0	0	0	0	0	0	0	0	-1	0	-2	-2	0	0	-2	0	4	1	0
liquid empty time	-29	3	0	0	15	0	0	0	-1	-1	0	0	78	300	3	-68	0	0	0	0	0	0	0	0	0	10	0	-8	0	0	0	6	0	-7	-64	0
liquid jet flow rate	1	0	0	0	-13	0	0	0	0	1	0	0	-44	-75	0	213	0	0	0	0	0	0	0	0	0	-10	0	9	0	0	0	-6	0	8	177	0
tank empty time	-28	3	0	0	8	0	0	0	3	2	0	0	78	207	-2	-47	0	0	0	0	0	0	0	0	0	13	0	-8	1	0	0	5	0	-5	-40	1
avg. jet flow rate	0	0	0	0	-8	0	0	0	-3	-2	0	0	-44	-67	2	87	0	0	0	0	0	0	0	0	0	-11	0	9	-1	0	0	-5	0	5	67	-1
plume diameter	0	0	-1	0	7	-1	0	0	-1	-1	0	0	-26	-49	1	6	-1	0	-10	0	0	0	0	0	0	1	0	3	-1	0	0	-1	-1	-2	4	-1
pool diameter	0	0	0	0	-6	0	0	0	0	0	0	0	-25	-50	0	76	0	0	0	0	0	12	0	0	0	10	0	5	0	0	0	-3	0	3	65	0
pool duration	-27	3	0	0	14	0	0	0	-1	-1	0	0	73	281	3	-64	-2	0	0	0	0	2	0	0	0	12	0	-8	0	0	0	4	0	-7	-60	0
max pool mass rate	1	0	0	0	-12	0	0	0	0	1	0	0	-44	-75	0	209	0	0	0	0	0	0	0	0	0	-10	0	9	0	0	0	-6	0	7	173	0
off-gassing duration	-25	3	0	0	13	0	0	0	-1	-1	0	0	70	273	3	-61	-2	0	0	0	0	3	0	0	0	13	0	-7	0	0	0	3	0	-7	-57	0
avg pool mass rate	-4	0	0	0	-11	0	0	0	0	1	0	0	-41	-73	0	155	3	0	0	0	0	-3	0	0	0	-12	0	8	0	0	0	-3	0	7	131	0
cloud diameter	-15	1	0	0	-15	0	0	0	-1	0	0	0	0	3	1	4	0	0	-10	15	0	0	0	0	0	16	0	-9	0	0	0	2	0	5	16	0
cloud temp	7	-3	18	0	66	14	0	0	4	0	0	0	-1	9	-36	13	-1	0	37	0	0	1	0	0	0	-25	0	32	13	0	0	-6	2	-11	-56	4
cloud duration	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
cloud vap mass rate	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Plume vapor source props																																				
diameter	0	0	-1	0	7	-1	0	0	-1	-1	0	0	-26	-49	1	6	-1	0	-10	0	0	0	0	0	0	1	0	3	-1	0	0	-1	-1	-2	4	-1
duration	-28	3	0	0	8	0	0	0	3	2	0	0	78	207	-2	-47	0	0	0	0	0	0	0	0	0	13	0	-8	1	0	0	5	0	-5	-40	1
vapor mass rate	0	0	0	0	-8	0	0	0	-3	-2	0	0	-44	-67	2	87	0	0	0	0	0	0	0	0	0	-11	0	9	-1	0	0	-5	0	5	67	-1

	25% Increase from Baseline Input Parameters																							25% Increase from Baseline Thermo Properties												
	itm	rc	at	gt	tt	h	tp	lhp	ihp	uvf	af	t	hd	od	lff	mfv	pd	pma	er	ch	fv	ws	sf	ft	ct	mw	lv	lhc	vhc	lst	vd	ld	ldr	bt	hov	hovr
final tank temp	-8	12	0	0	37	0	0	0	134	80	0	0	0		0	0	0	0	0	0	0	0	0	0	0	-105	0	0	-107	0	0	0	0	-96	0	0
depress. Temp	-1	1	0	0	29	0	0	0	0	-2	0	0	0		1	0	0	0	0	0	0	0	0	0	0	-5	0	4	0	0	0	4	0	1	-6	0
depress. Pressure	-1	1	0	0	6	0	0	0	3	3	0	0	0		1	0	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	1	0	-3	-2	0
liquid empty time	29	-3	0	0	-65	0	0	0	0	1	0	0	-36		-3	0	0	0	0	0	0	0	0	0	0	-7	0	8	0	0	0	-3	0	7	-7	0
liquid jet flow rate	0	0	0	0	187	0	0	0	0	-1	0	0	56		0	0	0	0	0	0	0	0	0	0	0	7	0	-7	0	0	0	3	0	-7	7	0
tank empty time	28	-3	0	0	-44	0	0	0	-2	-2	0	0	-36		3	0	0	0	0	0	0	0	0	0	0	-8	0	9	0	0	0	-3	1	6	-7	0
avg. jet flow rate	0	0	0	0	79	0	0	0	2	2	0	0	56		-3	0	0	0	0	0	0	0	0	0	0	8	0	-8	0	0	0	3	-1	-5	7	0
plume diameter	-1	-1	0	0	7	0	0	0	0	0	0	0	25		-1	0	0	0	9	0	0	-1	0	0	0	-2	0	-3	0	0	0	0	-1	1	1	-1
pool diameter	0	0	0	0	68	0	0	0	0	0	0	0	25		0	0	0	0	0	0	0	-9	0	0	0	-7	0	-4	0	0	0	2	0	-3	4	0
pool duration	27	-3	0	0	-61	0	0	0	0	1	0	0	-34		-3	0	1	0	0	0	0	-1	0	0	0	-8	0	7	0	0	0	-1	0	7	-6	0
max pool mass rate	0	0	0	0	182	0	0	0	0	-1	0	0	56		0	0	0	0	0	0	0	0	0	0	0	7	0	-8	0	0	0	3	0	-7	7	0
off-gassing duration	26	-3	0	0	-58	0	0	0	0	1	0	0	-32		-3	0	3	0	0	0	0	-2	0	0	0	-8	0	7	0	0	0	0	0	6	-6	0
avg pool mass rate	2	0	0	0	136	0	0	0	0	-1	0	0	47		0	0	-3	0	0	0	0	2	0	0	0	9	0	-7	0	0	0	0	0	-6	7	0
cloud diameter	13	-2	0	0	18	0	0	0	0	0	0	0	0		-1	0	0	0	9	-11	0	0	0	0	0	-11	0	8	0	0	0	-1	0	-6	-8	0
cloud temp	-4	4	-19	0	-26	-14	0	0	2	2	0	0	1		44	0	1	0	-25	0	0	0	0	0	0	24	0	-18	-10	0	0	2	4	22	74	2
cloud duration	0	0	0	0	0	0	0	0	0	0	0	0	0		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
cloud vap mass rate	0	0	0	0	0	0	0	0	0	0	0	0	0		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Plume vapor source props																																				
diameter	-1	-1	0	0	7	0	0	0	0	0	0	0	25		-1	0	0	0	9	0	0	-1	0	0	0	-2	0	-3	0	0	0	0	-1	1	1	-1
duration	28	-3	0	0	-44	0	0	0	-2	-2	0	0	-36		3	0	0	0	0	0	0	0	0	0	0	-8	0	9	0	0	0	-3	1	6	-7	0
vapor mass rate	0	0	0	0	79	0	0	0	2	2	0	0	56		-3	0	0	0	0	0	0	0	0	0	0	8	0	-8	0	0	0	3	-1	-5	7	0

Table B-7: Percentage Change Results Visualization:
High-Volatility Vignette – Hydrogen Sulfide

	25% Decrease from Baseline Input Parameters																							25% Decrease from Baseline Thermo Properties												
	itm	rc	at	gt	tt	h	tp	lhp	ihp	uvf	af	t	hd	od	lff	mfv	pd	pma	er	ch	fv	ws	sf	ft	ct	mw	lv	lhc	vhc	lst	vd	ld	ldr	bt	hov	hovr
final tank temp	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	4	0	0	4	0	0	0	0	21	0	0
depress. Temp	59	-48	0	0	-215	0	0	0	4	61	0	0	0	0	-21	0	0	0	0	0	0	0	0	0	0	221	0	-261	-4	0	0	-313	-31	-328	281	38
depress. Pressure	1	-1	0	0	-5	0	0	0	0	1	0	0	0	0	-1	0	0	0	0	0	0	0	0	0	0	5	0	-6	0	0	0	-7	-1	38	6	1
liquid empty time	-29	4	0	0	4	0	0	0	1	0	0	0	78	31	2	-7	0	0	0	0	0	0	0	0	0	7	0	4	0	0	0	11	1	-24	-4	0
liquid jet flow rate	0	0	0	0	-4	0	0	0	-1	0	0	0	-44	-24	0	7	0	0	0	0	0	0	0	0	0	-6	0	-2	0	0	0	-10	-1	28	2	0
tank empty time	-23	-2	0	0	3	0	0	0	0	-1	0	0	78	31	-7	-3	0	0	0	0	0	0	0	0	0	6	0	-3	0	0	0	11	1	-19	5	-1
avg. jet flow rate	-6	5	0	0	-3	0	0	0	0	1	0	0	-44	-23	7	3	0	0	0	0	0	0	0	0	0	-6	0	3	0	0	0	-10	-1	24	-5	1
plume diameter	0	0	0	0	-3	-1	0	0	0	0	-1	0	-25	-25	0	7	0	0	-13	0	0	0	0	0	0	12	0	-14	0	0	0	-9	-1	17	25	0
pool diameter	-15	2	0	0	1	0	0	0	0	0	-13	0	-2	-1	1	0	15	0	0	0	0	0	0	0	0	1	0	5	0	0	0	14	0	-5	-7	0
pool duration	-3	0	0	0	0	0	0	0	0	0	0	0	8	3	0	-1	-23	4	0	0	0	23	0	0	0	31	0	0	0	0	0	-21	0	-8	0	0
max pool mass rate	-28	4	0	0	1	0	0	0	0	0	-25	0	-4	-1	2	0	31	0	0	0	0	-20	0	0	0	-24	0	10	0	0	0	30	0	-3	-13	0
off-gassing duration	-2	0	0	0	0	0	0	0	0	0	0	0	5	2	0	0	-23	-7	0	0	0	24	0	0	0	32	0	0	0	0	0	-23	0	-8	0	0
avg pool mass rate	-28	4	0	0	1	0	0	0	0	0	-25	0	-5	-2	2	0	31	8	0	0	0	-20	0	0	0	-24	0	10	0	0	0	29	0	-2	-13	0
cloud diameter	-14	1	0	0	-2	0	0	0	0	0	0	0	-3	-1	0	0	0	0	-11	12	2	0	-1	0	0	19	0	-11	0	0	0	0	0	9	21	0
cloud temp	0	0	3	0	4	2	0	0	0	0	2	0	0	0	0	0	0	0	4	0	0	0	0	0	0	-25	0	4	1	0	0	0	0	-17	-51	0
cloud duration	-13	3	0	0	3	1	0	0	1	0	1	0	32	13	2	-3	0	0	9	-22	33	0	-15	0	0	-16	0	15	1	0	0	5	1	-17	-30	0
cloud vap mass rate	-17	0	0	0	-3	-1	0	0	-1	0	1	0	-24	-11	-2	4	0	0	-9	29	-25	0	17	0	0	19	0	-14	-1	0	0	-4	0	21	43	0
Plume vapor source prop																																				
diameter	0	0	0	0	-3	-1	0	0	0	0	-1	0	-25	-25	0	7	0	0	-13	0	0	0	0	0	0	12	0	-14	0	0	0	-9	-1	17	25	0
duration	-23	-2	0	0	3	0	0	0	0	-1	0	0	78	31	-7	-3	0	0	0	0	0	0	0	0	0	6	0	-3	0	0	0	11	1	-19	5	-1
vapor mass rate	-6	5	0	0	-3	0	0	0	0	1	0	0	-44	-23	7	3	0	0	0	0	0	0	0	0	0	-6	0	3	0	0	0	-10	-1	24	-5	1

	25% Increase from Baseline Input Parameters																							25% Increase from Baseline Thermo Properties												
	itm	rc	at	gt	tt	h	tp	lhp	ihp	uvf	af	t	hd	od	lff	mfv	pd	pma	er	ch	fv	ws	sf	ft	ct	mw	lv	lhc	vhc	lst	vd	ld	ldr	bt	hov	hovr
final tank temp	0	0	0	0	0	0	0	0	0	0	0	0	0		0	0	0	0	0	0	0	0	0	0	0	-3	0	0	-3	0	0	0	0	-20	0	0
depress. Temp	-36	44	0	0	214	0	0	0	-4	-68	0	0	0		23	0	0	0	0	0	0	0	0	0	0	-204	0	171	4	0	0	184	30	300	-254	-36
depress. Pressure	-1	1	0	0	5	0	0	0	0	-1	0	0	0		1	0	0	0	0	0	0	0	0	0	0	-4	0	4	0	0	0	4	1	-34	-5	-1
liquid empty time	29	-4	0	0	-4	0	0	0	-1	0	0	0	-36		-2	7	0	0	0	0	0	0	0	0	0	-4	0	-3	0	0	0	-7	-1	45	4	0
liquid jet flow rate	0	0	0	0	4	0	0	0	1	0	0	0	56		0	-6	0	0	0	0	0	0	0	0	0	4	0	2	0	0	0	7	1	-30	-2	0
tank empty time	23	2	0	0	-4	0	0	0	-1	1	0	0	-36		6	3	0	0	0	0	0	0	0	0	0	-4	0	4	0	0	0	-6	-1	37	-2	0
avg. jet flow rate	4	-4	0	0	4	0	0	0	1	-1	0	0	56		-6	-3	0	0	0	0	0	0	0	0	0	4	0	-4	0	0	0	7	1	-27	2	0
plume diameter	0	0	0	0	3	0	0	0	0	0	0	0	25		0	-6	0	0	14	0	0	0	0	3	0	-8	0	15	0	0	0	6	1	-19	-13	0
pool diameter	13	-2	0	0	-1	0	0	0	0	0	12	0	1		-1	0	-10	0	0	0	0	0	0	0	0	-1	0	-5	0	0	0	-10	0	4	4	0
pool duration	3	0	0	0	0	0	0	0	0	0	0	0	-4		0	1	22	-4	0	0	0	-15	0	0	0	-18	0	0	0	0	0	22	0	10	0	0
max pool mass rate	27	-4	0	0	-1	0	0	0	0	0	25	0	2		-2	0	-19	0	0	0	0	18	0	0	0	23	0	-10	0	0	0	-19	0	1	8	0
off-gassing duration	2	0	0	0	0	0	0	0	0	0	0	0	-2		0	0	23	7	0	0	0	-15	0	0	0	-19	0	0	0	0	0	23	0	9	0	0
avg pool mass rate	27	-4	0	0	-1	0	0	0	0	0	25	0	2		-2	0	-19	-7	0	0	0	18	0	0	0	23	0	-10	0	0	0	-19	0	1	8	0
cloud diameter	12	-1	0	0	2	0	0	0	0	0	0	0	1		0	0	0	0	14	-9	-3	0	1	4	0	-11	0	14	0	0	0	0	0	-7	-9	0
cloud temp	0	0	-3	0	-4	-2	0	0	0	0	-2	0	0		0	0	0	0	-20	0	0	0	0	-22	0	4	0	-26	-1	0	0	0	0	-7	4	0
cloud duration	13	-3	0	0	-3	-1	0	0	0	0	-1	0	-15		-2	3	0	0	-9	22	-24	0	15	-2	0	9	0	-14	0	0	0	-3	0	27	29	0
cloud vap mass rate	13	0	0	0	3	1	0	0	0	0	0	0	17		2	-3	0	0	10	-18	32	0	-13	2	0	-8	0	18	0	0	0	3	0	-21	-23	0
Plume vapor source prop																																				
diameter	0	0	0	0	3	0	0	0	0	0	0	0	25		0	-6	0	0	14	0	0	0	0	3	0	-8	0	15	0	0	0	6	1	-19	-13	0
duration	23	2	0	0	-4	0	0	0	-1	1	0	0	-36		6	3	0	0	0	0	0	0	0	0	0	-4	0	4	0	0	0	-6	-1	37	-2	0
vapor mass rate	4	-4	0	0	4	0	0	0	1	-1	0	0	56		-6	-3	0	0	0	0	0	0	0	0	0	4	0	-4	0	0	0	7	1	-27	2	0

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